Butyl 3-methoxypropionate
4195-88-4 | DTXSID30194709

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 191 °C

Global applicability domain: Inside

Local applicability domain index: 7.38e-01

Confidence level: 8.24e-01

Nearest Neighbors from the Training Set

Image not found
2-Butoxyethyl acetate
Measured: 192
Predicted: 191

Image not found
Butanoic anhydride
Measured: 200
Predicted: 194

Image not found
Diethylene glycol diethyl ether
Measured: 188
Predicted: 183

Image not found
Propane, 1,1,3,3-tetramethoxy-
Measured: 183
Predicted: 177

Image not found
Isobutyric anhydride
Measured: 183
Predicted: 185